

## REMARKS/ARGUMENTS

The office action issued October 6, 2004 continues the rejections of claim 1 under 35 U.S.C. 102(e) and, in addition, newly rejects claim 1 under 35 U.S.C. 102(b). Claims 2-7 were allowed.

### 35 U.S.C. 102(e) Rejection

Before proceeding, Applicants' attorney first wishes to thank Examiner Dougherty and Examiner Nghiem for the courtesies extended during the interview and for the productive discussion that resulted in agreement on the amendments necessary to place claim 1 in position for allowance over the 102(e) rejection. Previous to the interview, the Examiner and Applicants had exchanged differing views on the interpretation of the term "heterogeneous compound database" as employed in claim 1. With one small exception, claim 1 has been amended to incorporate the language modifying the term "heterogeneous compound database" as agreed upon and found in the Interview Summary of August 31, 2004. The one exception is the deletion of the word "whole" as modifying "molecule." Applicants respectfully submit that in the phrase "composed of whole molecules from different sources and syntheses, some known and some unknown", the use of the word "whole" is redundant. A molecule is a whole molecule. Unless one specifically talks about parts or fragments of a molecule as is done in the application, it is submitted that the normal understanding of the word "molecule" is understood to mean the entire or whole molecule.

In addition to the above noted amendment, amendment has also been made to claim 1

by replacing “defining fragments” with the term “fragmenting.” Applicants submit that with these amendments, claim 1 is now allowable over the 102(e) cited prior art.

35 U.S.C. 102(b) Rejection

The Examiner has rejected claim 1 under 35 U.S.C. 102(b): “... as being anticipated by International Application Publication Number WO 99/44055 to Nicholls.” Specifically, the Examiner states that Nicholls searches a heterogenous compound database with a method which uses the same steps as applicants’ method:

“...comprising the steps of defining fragments of a query molecule and a database molecule according to a defined set of rules (see page 11 line 8-27), generating shape descriptors for the query molecule and database molecule fragments (see page 22 line 10-19), and using the shape descriptors identifying the database molecule which has a shape similar to the query molecule (see page 23 line 5-26).”

Applicants respectfully disagree with the Examiner’s analysis for the following reasons. Initially, it is not clear whether the method of using ellipsoidal Gaussian decomposition to generate fragments of a molecule is equivalent to defining fragments according to a defined set of rules as that phrase is understood in light of the specification. However, for the present, applicants will not further address that issue because there is a clear distinction between the method of Nicholls and applicants’ invention. Specifically, even assuming arguendo that Nicholls teaches a method of generating fragments according to a defined set of rules, what Nicholls tries to accomplish with his fragment comparisons is different from what applicants

accomplish. Nicholls teaches that he can (shape) match subparts of one molecule with subparts of another molecule or that he can (shape) match a subpart of one molecule with another whole molecule. Nicholls is not concerned with finding a (shape) match of a whole query molecule to a whole database molecule using fragments. Yet, this is precisely what applicants teach. Applicants' method identifies the molecules in the heterogenous compound database which have the same shape as the query molecule by examining the shape comparisons between fragments of the query molecule and fragments of the database molecule. The method identifies the most similarly shaped database molecule as that molecule having the smallest field value differences in its fragments (compared to the fragments of the query molecule). In other words, applicants use fragments to compare whole molecules to whole molecules. This is the requirement of applicants' method stated in step 1.(c). For this reason, Nicholls can not anticipate applicants' invention. Accordingly, applicants respectfully request the Examiner to remove the 35 U.S.C. 102(b) rejection.

While claims 2-7 have been previously allowed, for consistency with claim 1, the language modifying "heterogeneous compound database" adopted in claim 1 has been further incorporated in claims 2, 3, and 6.

Finally, an RCE has been submitted since this is a response to a final office action.

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Respectfully submitted,



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